2,6-Dimethoxyamphetamine

Other names: Benzeneethanamine, 2,6-dimethoxy, «alpha»-methyl-
Inchi: InChI=1S/C11H17NO2/c1-8(12)7-9-10(13-2)5-4-6-11(9)14-3/h4-6,8H,7,12H2,1-3H3
InchiKey: OHGNLLDQBKOWJW-UHFFFAOYSA-N
Formula: C11H17NO2
SMILES: COc1cccc(OC)c1CC(C)N
Mol. weight [g/mol]: 195.26
CAS: 23690-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-11.10	kJ/mol	Joback Method
hf	-292.71	kJ/mol	Joback Method
hfus	21.56	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
ie	8.18 ± 0.06	eV	NIST Webbook
log10ws	-2.48		Crippen Method
logp	1.593		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2651.56	kPa	Joback Method
tb	604.65	K	Joback Method
tc	818.55	K	Joback Method
tf	377.91	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.34	J/mol×K	604.65	Joback Method
cpg	428.28	J/mol×K	640.30	Joback Method
cpg	442.45	J/mol×K	675.95	Joback Method
cpg	455.85	J/mol×K	711.60	Joback Method
cpg	468.48	J/mol×K	747.25	Joback Method
cpg	480.33	J/mol×K	782.90	Joback Method
cpg	491.41	J/mol×K	818.55	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23690144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume